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\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	DEC 01	ChemPort single article sales feature unavailable
NEWS	3	FEB 02	Simultaneous left and right truncation (SLART) added for CERAB, COMPUAB, ELCOM, and SOLIDSTATE
NEWS	4	FEB 02	GENBANK enhanced with SET PLURALS and SET SPELLING
NEWS	5	FEB 06	Patent sequence location (PSL) data added to USGENE
NEWS	6	FEB 10	COMPENDEX reloaded and enhanced
NEWS	7	FEB 11	WTEXTILES reloaded and enhanced
NEWS	8	FEB 19	New patent-examiner citations in 300,000 CA/CAPLUS patent records provide insights into related prior art
NEWS	9	FEB 19	Increase the precision of your patent queries -- use terms from the IPC Thesaurus, Version 2009.01
NEWS	10	FEB 23	Several formats for image display and print options discontinued in USPATFULL and USPAT2
NEWS	11	FEB 23	MEDLINE now offers more precise author group fields and 2009 MeSH terms
NEWS	12	FEB 23	TOXCENTER updates mirror those of MEDLINE - more precise author group fields and 2009 MeSH terms
NEWS	13	FEB 23	Three million new patent records blast AEROSPACE into STN patent clusters
NEWS	14	FEB 25	USGENE enhanced with patent family and legal status display data from INPADOCDB
NEWS	15	MAR 06	INPADOCDB and INPAFAMDB enhanced with new display formats
NEWS	16	MAR 11	EPFULL backfile enhanced with additional full-text applications and grants
NEWS	17	MAR 11	ESBIOBASE reloaded and enhanced
NEWS	18	MAR 20	CAS databases on STN enhanced with new super role for nanomaterial substances
NEWS	19	MAR 23	CA/CAPLUS enhanced with more than 250,000 patent equivalents from China
NEWS	20	MAR 30	IMSPATENTS reloaded and enhanced
NEWS	21	APR 03	CAS coverage of exemplified prophetic substances enhanced
NEWS	22	APR 07	STN is raising the limits on saved answers
NEWS	23	APR 24	CA/CAPLUS now has more comprehensive patent assignee information
NEWS	24	APR 26	USPATFULL and USPAT2 enhanced with patent assignment/reassignment information
NEWS	25	APR 28	CAS patent authority coverage expanded
NEWS	26	APR 28	ENCOMPLIT/ENCOMPLIT2 search fields enhanced
NEWS	27	APR 28	Limits doubled for structure searching in CAS REGISTRY

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,

AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 20:33:38 ON 06 MAY 2009

=> file retg  
'RETG' IS NOT A VALID FILE NAME  
SESSION CONTINUES IN FILE 'HOME'  
Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files that are available. If you have requested multiple files, you can specify a corrected file name or you can enter "IGNORE" to continue accessing the remaining file names entered.

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.22	0.22

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STRUCTURE FILE UPDATES:    5 MAY 2009    HIGHEST RN 1143038-16-7  
DICTIONARY FILE UPDATES:   5 MAY 2009    HIGHEST RN 1143038-16-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

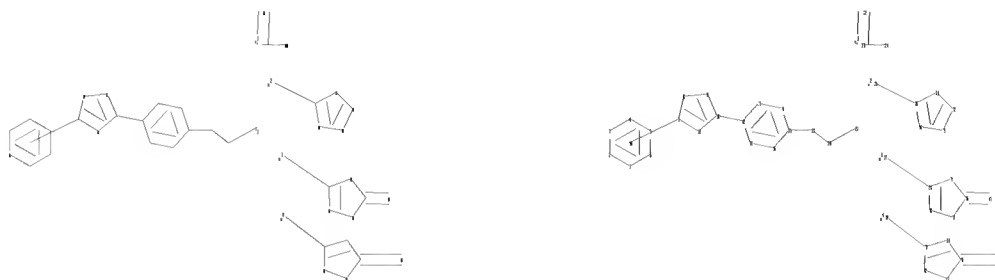
TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>  
Uploading C:\Program Files\STNEXP\Queries\10575790dd.str



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chain nodes :
21 22 23 24 25 27 29 43 44
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 26 28 30 31 32 33
34 35 36 37 38 39 40 41 42
ring/chain nodes :
18 20
chain bonds :
10-12 15-18 18-20 20-21 22-23 23-24 25-26 27-28 29-30 36-43 40-44
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-11 7-8 8-9 9-10 10-11 12-13 12-17 13-14
14-15 15-16 16-17 26-31 26-34 28-35 28-38 30-39 30-42 31-32 32-33 33-34
35-36 36-37 37-38 39-40 40-41 41-42
exact/norm bonds :
7-11 9-10 10-11 20-21 26-31 26-34 28-35 28-38 30-39 30-42 31-32 32-33
33-34 35-36 36-37 36-43 37-38 39-40 40-41 40-44 41-42
exact bonds :
7-8 8-9 10-12 15-18 18-20 25-26 27-28 29-30
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 12-13 12-17 13-14 14-15 15-16 16-17 22-23
23-24
isolated ring systems :
containing 1 : 7 : 12 :

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G1:[*1],[*2],[*3],[*4]

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Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 20:CLASS
21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:Atom 27:CLASS 28:Atom
29:CLASS 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom
38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:CLASS 44:CLASS 50:Atom

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L1        STRUCTURE UPLOADED

=> s l1 sss full

FULL SEARCH INITIATED 20:34:28 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED -        74 TO ITERATE

100.0% PROCESSED        74 ITERATIONS

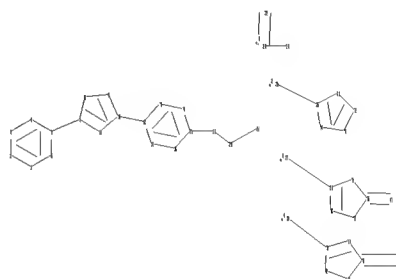
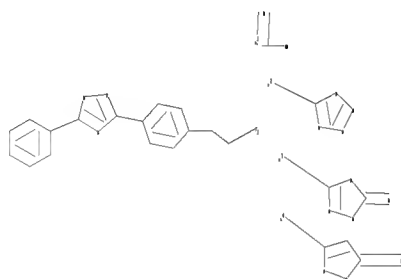
37 ANSWERS

SEARCH TIME: 00.00.01

L2        37 SEA SSS FUL L1

=>

Uploading C:\Program Files\STNEXP\Queries\10575790cc.str



chain nodes :

21 22 23 24 25 27 29 43 44

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 26 28 30 31 32 33  
34 35 36 37 38 39 40 41 42

ring/chain nodes :

18 20

chain bonds :

5-7 10-12 15-18 18-20 20-21 22-23 23-24 25-26 27-28 29-30 36-43 40-44

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11 12-13 12-17 13-14  
14-15 15-16 16-17 26-31 26-34 28-35 28-38 30-39 30-42 31-32 32-33 33-34  
35-36 36-37 37-38 39-40 40-41 41-42

exact/norm bonds :  
7-11 9-10 10-11 20-21 26-31 26-34 28-35 28-38 30-39 30-42 31-32 32-33  
33-34 35-36 36-37 36-43 37-38 39-40 40-41 40-44 41-42  
exact bonds :  
5-7 7-8 8-9 10-12 15-18 18-20 25-26 27-28 29-30  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6 12-13 12-17 13-14 14-15 15-16 16-17 22-23  
23-24  
isolated ring systems :  
containing 1 : 7 : 12 :

G1:[\*1],[\*2],[\*3],[\*4]

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 20:CLASS  
21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:Atom 27:CLASS 28:Atom  
29:CLASS 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom  
38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:CLASS 44:CLASS

L3 STRUCTURE UPLOADED

=> s l3 sss full  
FULL SEARCH INITIATED 20:34:48 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 224 TO ITERATE

100.0% PROCESSED 224 ITERATIONS 38 ANSWERS  
SEARCH TIME: 00.00.01

L4 38 SEA SSS FUL L3

=> file capl  
COST IN U.S. DOLLARS SINCE FILE TOTAL  
ENTRY SESSION  
FULL ESTIMATED COST 371.76 371.98

FILE 'CAPLUS' ENTERED AT 20:34:51 ON 06 MAY 2009  
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FILE COVERS 1907 - 6 May 2009 VOL 150 ISS 19  
FILE LAST UPDATED: 5 May 2009 (20090505/ED)  
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2009  
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2009

Caplus now includes complete International Patent Classification (IPC)

reclassification data for the third quarter of 2008.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 12

L5 6 L2

=> s 14

L6 5 L4

=> s 15 or 16

L7 8 L5 OR L6

=> d 17 1-8 ibib hitstr

L7 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:1158632 CAPLUS

DOCUMENT NUMBER: 149:402366

TITLE: Preparation of aminopyridine derivatives, particularly 3-(aminopyridinyl)-5-(alkoxyphenyl)-1,2,4-oxadiazoles, as immunomodulating S1P1/EDG1 receptor agonists

INVENTOR(S): Bolli, Martin; Mathys, Boris; Mueller, Claus; Nayler, Oliver; Steiner, Beat; Velker, Joerg

PATENT ASSIGNEE(S): Actelion Pharmaceuticals Ltd, Switz.

SOURCE: PCT Int. Appl., 121pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008114157	A1	20080925	WO 2008-IB50742	20080229
W:	AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			

PRIORITY APPLN. INFO.: WO 2007-IB50921 A 20070316

OTHER SOURCE(S): MARPAT 149:402366

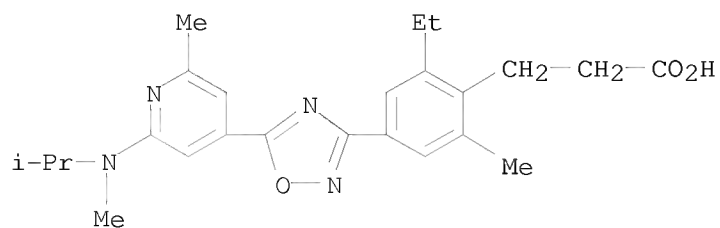
IT 1062670-28-3P, 3-[2-Ethyl-4-[5-[2-[(isopropyl)(methyl)amino]-6-methylpyridin-4-yl][1,2,4]oxadiazol-3-yl]-6-methylphenyl]propionic acid

1062670-96-5P, 3-[4-[5-(2-Diethylamino-6-methylpyridin-4-yl)[1,2,4]oxadiazol-3-yl]-2-ethyl-6-methylphenyl]propionic acid

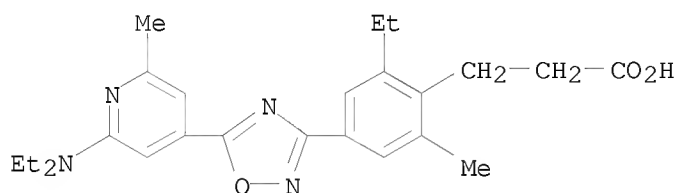
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(drug candidate; preparation of aminopyridine derivs. as immunomodulating S1P1/EDG1 receptor agonists)

RN 1062670-28-3 CAPLUS  
 CN Benzenepropanoic acid, 2-ethyl-6-methyl-4-[5-[2-methyl-6-[methyl(1-methylethyl)amino]-4-pyridinyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)

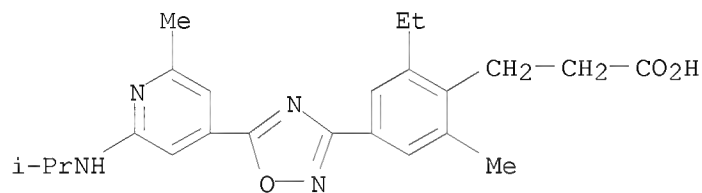


RN 1062670-96-5 CAPLUS  
 CN Benzenepropanoic acid, 4-[5-[2-(diethylamino)-6-methyl-4-pyridinyl]-1,2,4-oxadiazol-3-yl]-2-ethyl-6-methyl- (CA INDEX NAME)



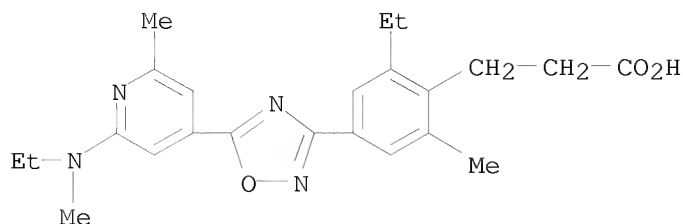
IT 1062673-09-9P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (drug candidate; preparation of aminopyridine derivs. as immunomodulating S1P1/EDG1 receptor agonists)

RN 1062673-09-9 CAPLUS  
 CN Benzenepropanoic acid, 2-ethyl-6-methyl-4-[5-[2-methyl-6-[(1-methylethyl)amino]-4-pyridinyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)

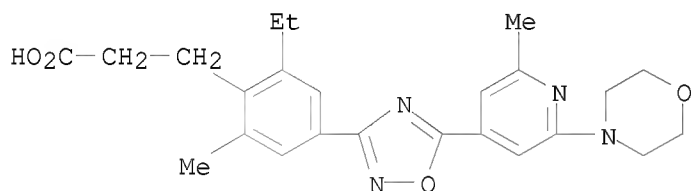


IT 1062669-77-5P, 3-[2-Ethyl-4-[5-[2-[(ethyl)(methyl)amino]-6-methylpyridin-4-yl][1,2,4]oxadiazol-3-yl]-6-methylphenyl]propionic acid  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (drug candidate; preparation of aminopyridine derivs. as immunomodulating S1P1/EDG1 receptor agonists)

RN 1062669-77-5 CAPLUS  
 CN Benzenepropanoic acid, 2-ethyl-4-[5-[2-(ethylmethylamino)-6-methyl-4-pyridinyl]-1,2,4-oxadiazol-3-yl]-6-methyl- (CA INDEX NAME)



IT 1062673-25-9P, 3-[2-Ethyl-6-methyl-4-[5-[2-methyl-6-(morpholin-4-yl)pyridin-4-yl][1,2,4]oxadiazol-3-yl]phenyl]propionic acid  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of aminopyridine derivs. as immunomodulating SlP1/EDG1 receptor agonists)  
 RN 1062673-25-9 CAPLUS  
 CN Benzenepropanoic acid, 2-ethyl-6-methyl-4-[5-[2-methyl-6-(4-morpholinyl)-4-pyridinyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2008:411236 CAPLUS  
 DOCUMENT NUMBER: 148:403230  
 TITLE: Preparation of diaryloxadiazole derivatives for use as antiinflammatory and immunosuppressive agents  
 INVENTOR(S): Albert, Rainer; Cooke, Nigel Graham; Lewis, Ian; Weiler, Sven; Zecri, Frederic  
 PATENT ASSIGNEE(S): Novartis A.-G., Switz.  
 SOURCE: PCT Int. Appl., 35pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008037476	A1	20080403	WO 2007-EP8431	20070927
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GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,  
 BY, KG, KZ, MD, RU, TJ, TM  
 AU 2007302262 A1 20080403 AU 2007-302262 20070927  
 PRIORITY APPLN. INFO.: EP 2006-121495 A 20060929  
 WO 2007-EP8431 W 20070927

OTHER SOURCE(S): MARPAT 148:403230

IT 1016261-25-8P 1016261-26-9P

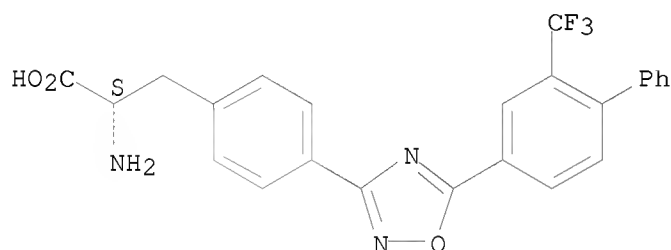
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)

(preparation of diaryloxadiazole derivs. for use as antiinflammatory and  
 immunosuppressive agents)

RN 1016261-25-8 CAPLUS

CN L-Phenylalanine, 4-[5-[2-(trifluoromethyl)[1,1'-biphenyl]-4-yl]-1,2,4-  
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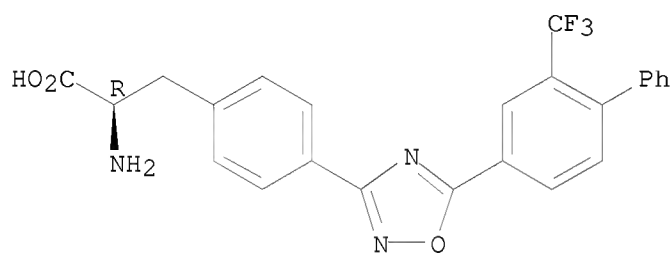
Absolute stereochemistry.



RN 1016261-26-9 CAPLUS

CN D-Phenylalanine, 4-[5-[2-(trifluoromethyl)[1,1'-biphenyl]-4-yl]-1,2,4-  
 oxadiazol-3-yl]- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:322210 CAPLUS

DOCUMENT NUMBER: 148:355634

TITLE: Pyridin-3-yl derivatives as immunomodulating agents  
 and their preparation, pharmaceutical compositions and  
 use in the treatment of immune system disorders

INVENTOR(S): Bolli, Martin; Lehmann, David; Mathys, Boris; Mueller,  
 Claus; Nayler, Oliver; Steiner, Beat; Velker, Joerg

PATENT ASSIGNEE(S): Actelion Pharmaceuticals Ltd., Switz.

SOURCE: PCT Int. Appl., 82pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008029370	A1	20080313	WO 2007-IB53593	20070906
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PRIORITY APPLN. INFO.:

WO 2006-IB53187 A 20060908

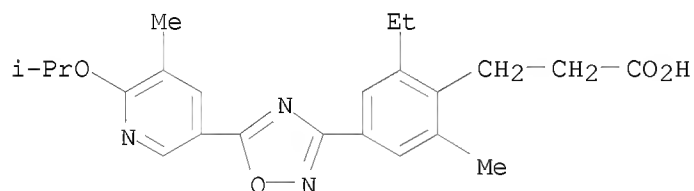
OTHER SOURCE(S): MARPAT 148:355634

IT 1011476-25-7P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(drug candidate and intermediate; preparation of pyridinyl derivs. as immunomodulating agents useful in the treatment of immune system disorders)

RN 1011476-25-7 CAPLUS

CN Benzenepropanoic acid, 2-ethyl-6-methyl-4-[5-[5-methyl-6-(1-methylethoxy)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:322202 CAPLUS

DOCUMENT NUMBER: 148:331565

TITLE: Pyridin-4-yl derivatives as immunomodulating agents and their preparation, pharmaceutical compositions and use in the treatment of immune system disorders

INVENTOR(S): Bolli, Martin; Lehmann, David; Mathys, Boris; Mueller, Claus; Nayler, Oliver; Steiner, Beat; Velker, Joerg

PATENT ASSIGNEE(S): Actelion Pharmaceuticals Ltd., Switz.

SOURCE: PCT Int. Appl., 132pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2008029371 A1 20080313 WO 2007-IB53594 20070906  
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GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG,  
KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME,  
MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL,  
PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN,  
TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW  
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,  
IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF,  
BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW,  
GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,  
BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: WO 2006-IB53147 A 20060907  
OTHER SOURCE(S): MARPAT 148:331565

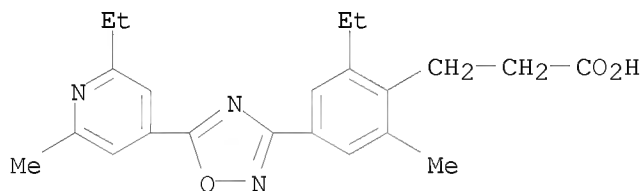
IT 1011264-28-0P 1011264-30-4P 1011264-32-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(intermediate; preparation of pyridinyl derivs. as immunomodulating agents  
useful in the treatment of immune system disorders)

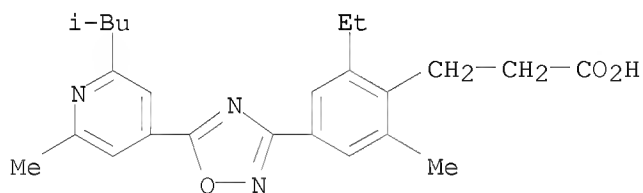
RN 1011264-28-0 CAPLUS

CN Benzenepropanoic acid, 2-ethyl-4-[5-(2-ethyl-6-methyl-4-pyridinyl)-1,2,4-  
oxadiazol-3-yl]-6-methyl- (CA INDEX NAME)



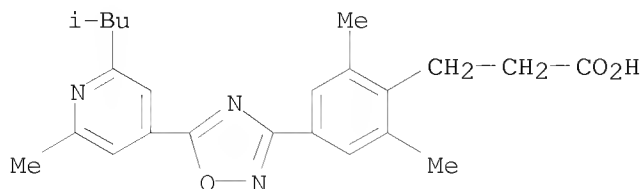
RN 1011264-30-4 CAPLUS

CN Benzenepropanoic acid, 2-ethyl-6-methyl-4-[5-[2-methyl-6-(2-methylpropyl)-  
4-pyridinyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)



RN 1011264-32-6 CAPLUS

CN Benzenepropanoic acid, 2,6-dimethyl-4-[5-[2-methyl-6-(2-methylpropyl)-4-  
pyridinyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:81270 CAPLUS

DOCUMENT NUMBER: 146:337810

TITLE: SAR studies of 3-arylpropionic acids as potent and selective agonists of sphingosine-1-phosphate receptor-1 (S1P1) with enhanced pharmacokinetic properties

AUTHOR(S): Yan, Lin; Huo, Pei; Hale, Jeffrey J.; Mills, Sander G.; Hajdu, Richard; Keohane, Carol A.; Rosenbach, Mark J.; Milligan, James A.; Shei, Gan-Ju; Chrebet, Gary; Bergstrom, James; Card, Deborah; Mandala, Suzanne M.

CORPORATE SOURCE: Department of Medicinal Chemistry, Merck Research Laboratories, Rahway, NJ, 07065, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2007), 17(3), 828-831

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 146:337810

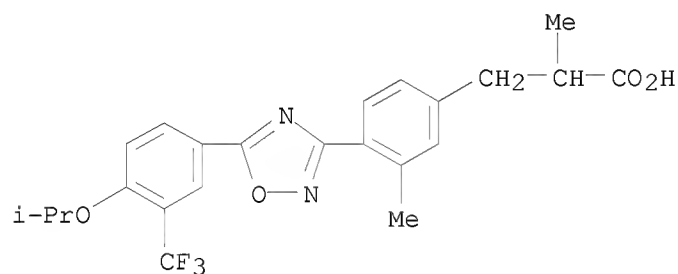
IT 856166-23-9P 856166-26-2P

RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation, sphingosinephosphate receptor agonistic activity, pharmacokinetics, and structure-activity relationship of (oxadiazolylaryl)propionic acids using Heck coupling reaction)

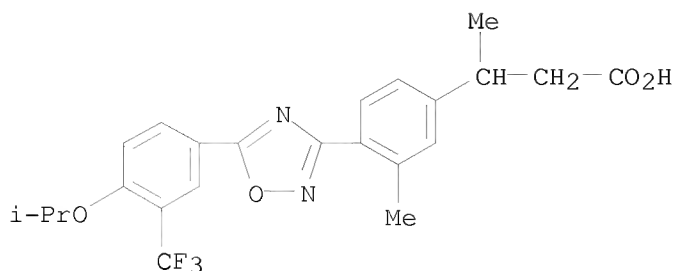
RN 856166-23-9 CAPLUS

CN Benzenepropanoic acid,  $\alpha$ ,3-dimethyl-4-[5-[4-(1-methylethoxy)-3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)



RN 856166-26-2 CAPLUS

CN Benzenepropanoic acid,  $\beta$ ,3-dimethyl-4-[5-[4-(1-methylethoxy)-3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2006:548763 CAPLUS

DOCUMENT NUMBER: 145:180190

TITLE: Highly selective and potent agonists of sphingosine-1-phosphate 1 (S1P1) receptor

AUTHOR(S): Vachal, Petr; Toth, Leslie M.; Hale, Jeffrey J.; Yan, Lin; Mills, Sander G.; Chrebet, Gary L.; Koehane, Carol A.; Hajdu, Richard; Milligan, James A.; Rosenbach, Mark J.; Mandala, Suzanne

CORPORATE SOURCE: Department of Medicinal Chemistry, Merck & Co., Inc., Rahway, NJ, 07065, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2006), 16(14), 3684-3687

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

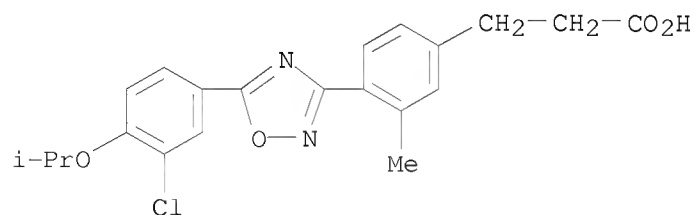
IT 856166-11-5P 856166-29-5P 856167-04-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(agonists of sphingosine-1-phosphate 1 receptor)

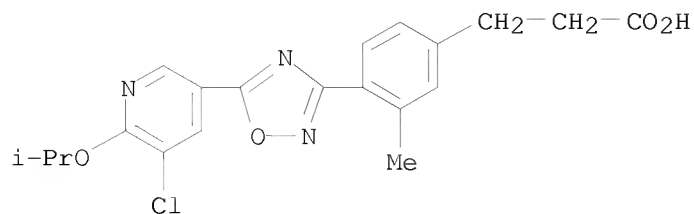
RN 856166-11-5 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-chloro-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

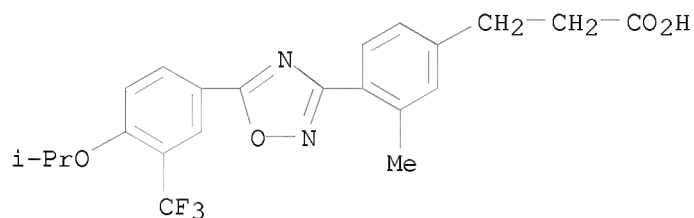


RN 856166-29-5 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-chloro-6-(1-methylethoxy)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



RN 856167-04-9 CAPLUS  
 CN Benzenepropanoic acid, 3-methyl-4-[5-[4-(1-methylethoxy)-3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2006:548762 CAPLUS

DOCUMENT NUMBER: 145:210970

TITLE: Discovery of 3-arylpropionic acids as potent agonists of sphingosine-1-phosphate receptor-1 (S1P1) with high selectivity against all other known S1P receptor subtypes

AUTHOR(S): Yan, Lin; Huo, Pei; Doherty, George; Toth, Lesile; Hale, Jeffrey J.; Mills, Sander G.; Hajdu, Richard; Keohane, Carol A.; Rosenbach, Mark J.; Milligan, James A.; Shei, Gan-Ju; Chrebet, Gary; Bergstrom, James; Card, Deborah; Quackenbush, Elizabeth; Wickham, Alexandra; Mandala, Suzanne M.

CORPORATE SOURCE: Department of Medicinal Chemistry, Merck Research Laboratories, Rahway, NJ, 07065, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2006), 16(14), 3679-3683

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 145:210970

IT 856166-09-1P 856166-11-5P 856166-12-6P

856166-13-7P 856166-14-8P 856166-15-9P

856166-16-0P 856166-29-5P 856166-34-2P

856166-74-0P 856166-82-0P 856166-88-6P

856166-89-7P 856166-90-0P 856167-04-9P

905308-11-4P 905308-18-1P 905308-20-5P

905308-32-9P 905308-36-3P 905308-38-5P

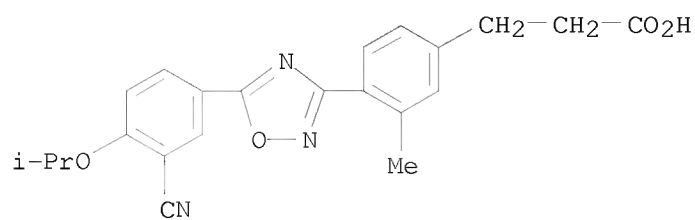
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL

(Biological study); PREP (Preparation)

(discovery of 3-arylpropionic acids as potent agonists of sphingosine-1-phosphate receptor-1 (S1P1) with high selectivity against all other known S1P receptor subtypes)

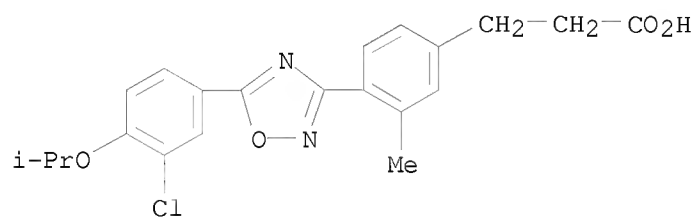
RN 856166-09-1 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-cyano-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



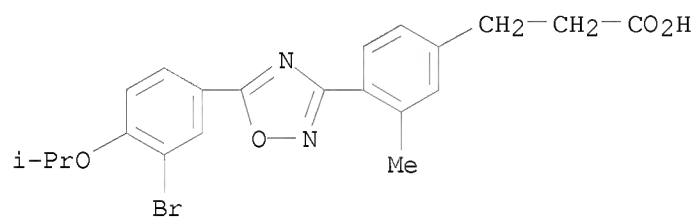
RN 856166-11-5 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-chloro-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



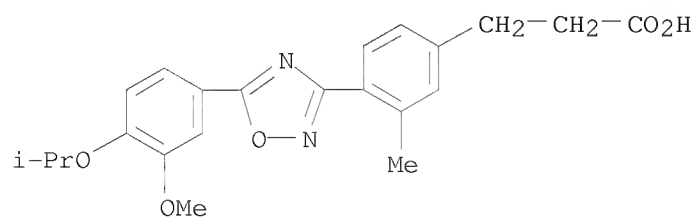
RN 856166-12-6 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-bromo-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



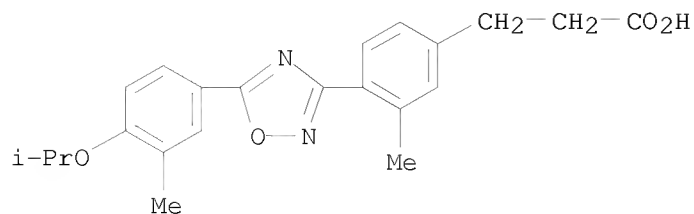
RN 856166-13-7 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-methoxy-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



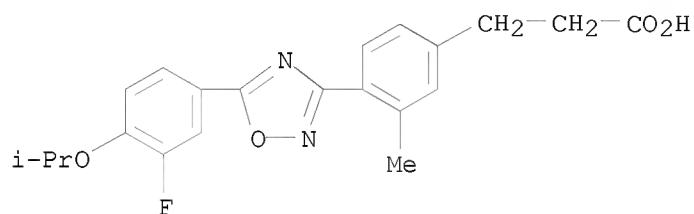
RN 856166-14-8 CAPLUS

CN Benzenepropanoic acid, 3-methyl-4-[5-[3-methyl-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)



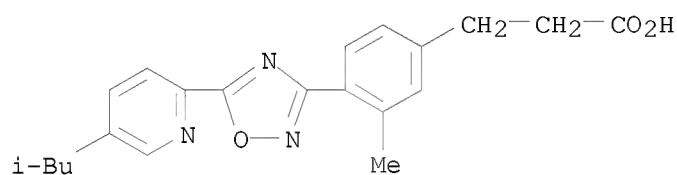
RN 856166-15-9 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-fluoro-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



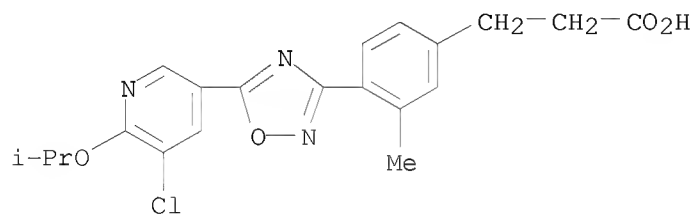
RN 856166-16-0 CAPLUS

CN Benzenepropanoic acid, 3-methyl-4-[5-[5-(2-methylpropyl)-2-pyridinyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)



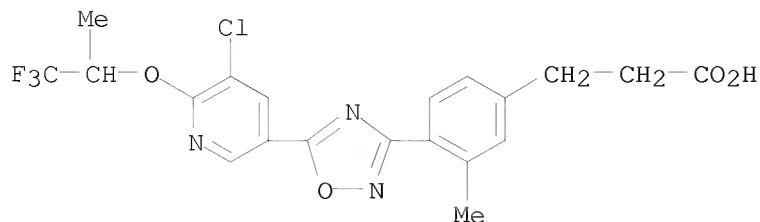
RN 856166-29-5 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-chloro-6-(1-methylethoxy)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



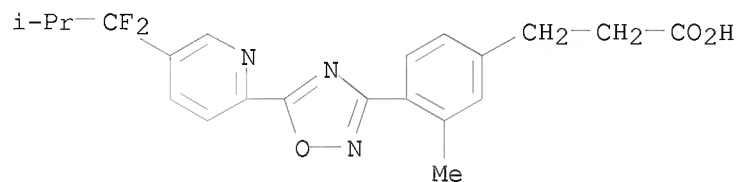
RN 856166-34-2 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-chloro-6-(2,2,2-trifluoro-1-methylethoxy)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



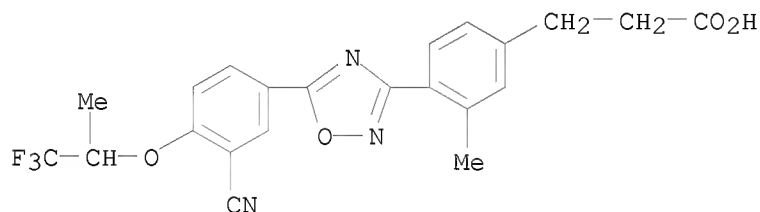
RN 856166-74-0 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-(1,1-difluoro-2-methylpropyl)-2-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



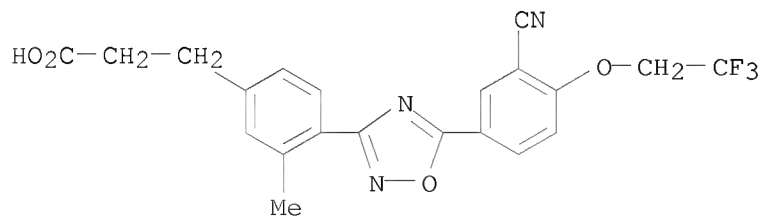
RN 856166-82-0 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-cyano-4-(2,2,2-trifluoro-1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



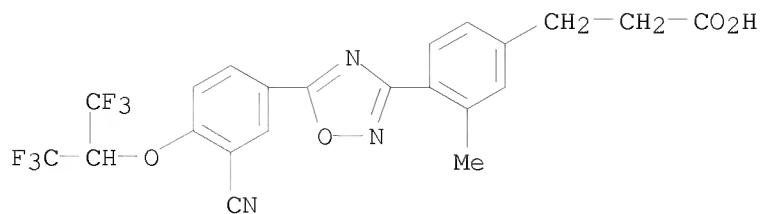
RN 856166-88-6 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-cyano-4-(2,2,2-trifluoroethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



RN 856166-89-7 CAPLUS

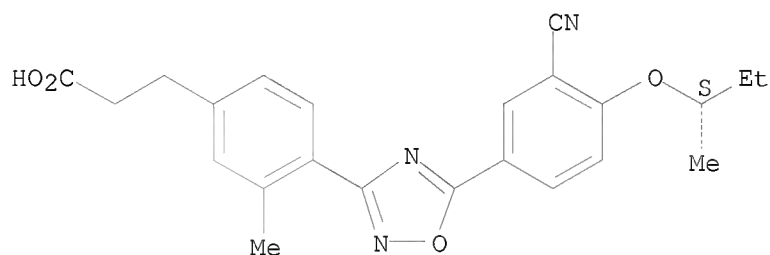
CN Benzenepropanoic acid, 4-[5-[3-cyano-4-[2,2,2-trifluoro-1-(trifluoromethyl)ethoxy]phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



RN 856166-90-0 CAPLUS

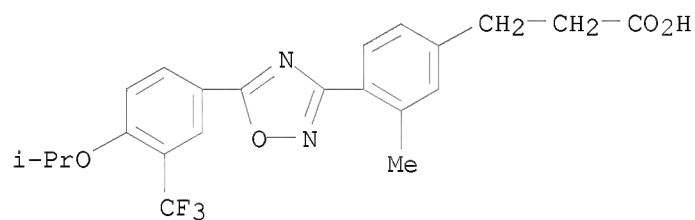
CN Benzenepropanoic acid, 4-[5-[3-cyano-4-[(1S)-1-methylpropoxy]phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

Absolute stereochemistry.



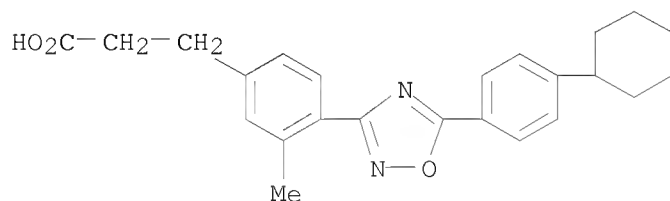
RN 856167-04-9 CAPLUS

CN Benzenepropanoic acid, 3-methyl-4-[5-[4-(1-methylethoxy)-3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)



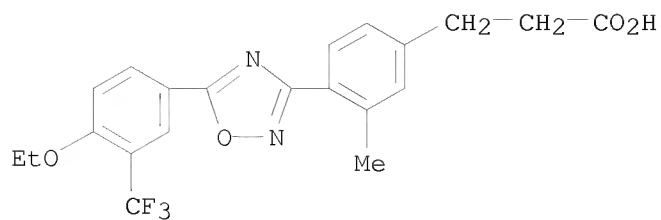
RN 905308-11-4 CAPLUS

CN Benzenepropanoic acid, 4-[5-(4-cyclohexylphenyl)-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



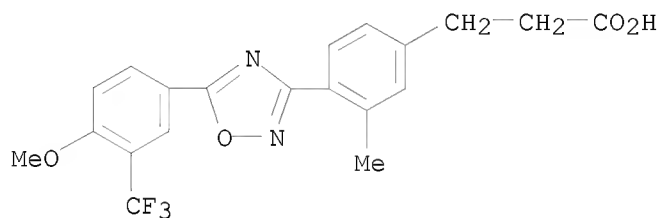
RN 905308-18-1 CAPLUS

CN Benzenepropanoic acid, 4-[5-[4-ethoxy-3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



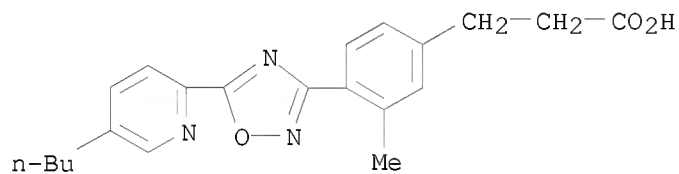
RN 905308-20-5 CAPLUS

CN Benzenepropanoic acid, 4-[5-[4-methoxy-3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



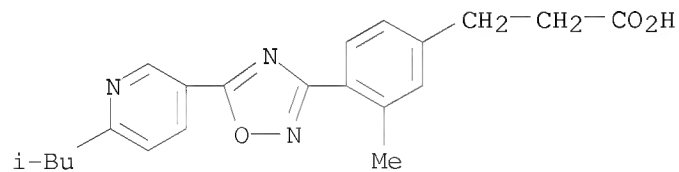
RN 905308-32-9 CAPLUS

CN Benzenepropanoic acid, 4-[5-(5-butyl-2-pyridinyl)-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



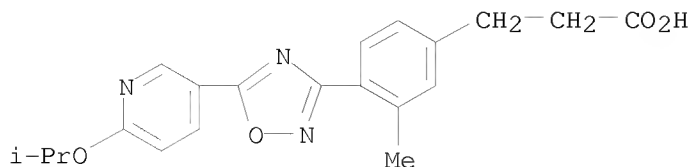
RN 905308-36-3 CAPLUS

CN Benzenepropanoic acid, 3-methyl-4-[5-[6-(2-methylpropyl)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)



RN 905308-38-5 CAPLUS

CN Benzenepropanoic acid, 3-methyl-4-[5-[6-(1-methylethoxy)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:564648 CAPLUS

DOCUMENT NUMBER: 143:97368

TITLE: Preparation of five-membered heterocycle-substituted benzenepropanoic and related acids as selective S1P1 (EDG1) receptor agonists

INVENTOR(S): Colandrea, Vincent J.; Doherty, George A.; Hale, Jeffrey J.; Huo, Pei; Legiec, Irene E.; Toth, Leslie; Vachal, Petr; Yan, Lin

PATENT ASSIGNEE(S): Merck & Co., Inc., USA

SOURCE: PCT Int. Appl., 230 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005058848	A1	20050630	WO 2004-US41887	20041213
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, VZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004299456	A1	20050630	AU 2004-299456	20041213
CA 2547198	A1	20050630	CA 2004-2547198	20041213
EP 1697333	A1	20060906	EP 2004-814111	20041213
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				
CN 1894225	A	20070110	CN 2004-80037208	20041213
JP 2007515432	T	20070614	JP 2006-545810	20041213
US 20080249093	A1	20081009	US 2006-575790	20060412
IN 2006DN02136	A	20070629	IN 2006-DN2136	20060419
PRIORITY APPLN. INFO.:			US 2003-530186P	P 20031217
			WO 2004-US41887	W 20041213

OTHER SOURCE(S): CASREACT 143:97368; MARPAT 143:97368

IT 856166-09-1P, 3-[4-[5-(3-Cyano-4-isopropoxyphenyl)-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-11-5P, 3-[4-[5-(4-Isopropoxy-3-chlorophenyl)-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-12-6P, 3-[4-[5-(4-Isopropoxy-3-bromophenyl)-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-13-7P, 3-[4-[5-(4-Isopropoxy-3-methoxyphenyl)-1,2,4-oxadiazol-3-yl]-3-

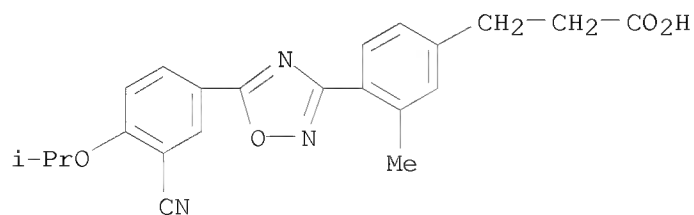
methylphenyl]propanoic acid 856166-14-8P,  
3-[4-[5-(4-Isopropoxy-3-methylphenyl)-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-15-9P,  
3-[4-[5-(4-Isopropoxy-3-fluorophenyl)-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-16-0P,  
3-[4-[5-[5-(2-Methylpropyl)pyridin-2-yl]-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-23-9P,  
2-Methyl-3-[4-[5-[3-(trifluoromethyl)-4-isopropoxyphenyl]-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-24-0P,  
2-Methyl-3-[4-[5-(3-cyano-4-isopropoxyphenyl)-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-25-1P,  
2-Methyl-3-[4-[5-(3-methyl-4-isopropoxyphenyl)-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-26-2P,  
3-[4-[5-[3-(Trifluoromethyl)-4-isopropoxyphenyl]-1,2,4-oxadiazol-3-yl]-3-methylphenyl]butanoic acid 856166-27-3P,  
3-[4-[5-(3-Cyano-4-isopropoxyphenyl)-1,2,4-oxadiazol-3-yl]-3-methylphenyl]butanoic acid 856166-28-4P,  
3-[4-[5-(3-Methyl-4-isopropoxyphenyl)-1,2,4-oxadiazol-3-yl]-3-methylphenyl]butanoic acid 856166-29-5P,  
3-[4-[5-(5-Chloro-6-isopropoxy-pyridin-3-yl)-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-32-0P,  
3-[4-[5-(5-Chloro-6-isopropylaminopyridin-3-yl)-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-34-2P,  
3-[4-[5-[5-Chloro-6-[1-(trifluoromethyl)ethoxy]pyridin-3-yl]-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-35-3P,  
3-[4-[5-[5-Chloro-6-(pyrrolidin-1-yl)pyridin-3-yl]-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-36-4P,  
3-[4-[5-[5-Chloro-6-(morpholin-4-yl)pyridin-3-yl]-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-37-5P,  
3-[4-[5-[5-Chloro-6-[(isopropyl)(methyl)amino]pyridin-3-yl]-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-38-6P,  
3-[4-[5-[5-Chloro-6-(2,2,2-trifluoroethoxy)pyridin-3-yl]-1,2,4-oxadiazol-3-yl]-3-methylphenyl]butanoic acid 856166-39-7P,  
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3-[4-[5-[5-Chloro-6-(3,3-difluoropiperidin-1-yl)pyridin-3-yl]-1,2,4-oxadiazol-3-yl]-3-methylphenyl]butanoic acid 856166-41-1P,  
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3-[4-[5-(5-Chloro-6-isobutylpyridin-3-yl)-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-50-2P,  
3-[4-[5-[5-Iodo-6-(N-isopropyl-N-methylamino)pyridin-3-yl]-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-51-3P,  
3-[4-[5-[5-Cyano-6-(N-isopropyl-N-methylamino)pyridin-3-yl]-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-54-6P,  
3-[4-[5-[6-(3,3-Difluoropyrrolidin-1-yl)-5-iodopyridin-3-yl]-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-55-7P,  
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3-[4-[5-(5-Cyano-6-ethoxypyridin-3-yl)-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-76-2P,  
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3-[4-[5-[4-(1,1-Difluoro-2-methylpropyl)phenyl]-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-79-5P,  
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3-yl]-3-methylphenyl]propanoic acid 856166-80-8P,  
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 3-[4-[5-[3-Cyano-4-[1-(trifluoromethyl)ethoxy]phenyl]-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-83-1P,  
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 3-[4-[5-(3,5-Dichloro-4-isopropoxyphenyl)-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-85-3P,  
 3-[4-[5-[3-Chloro-4-(cyclopropylmethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-86-4P 856166-87-5P,  
 3-[4-[5-[3-Nitro-4-[1-(trifluoromethyl)ethoxy]phenyl]-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-88-6P,  
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 , 3-[4-[5-[3-Cyano-4-[(S)-1-methylpropyl]oxy]phenyl]-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-91-1P,  
 3-[4-[5-[4-(Trifluoromethyl)-6-[1-(trifluoromethyl)ethoxy]pyridin-3-yl]-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-92-2P  
 , 3-[4-[5-[4-Amino-6-(2,2,2-trifluoro-1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-94-4P,  
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 3-[4-[5-[3-Cyano-4-[1-(trifluoromethyl)-2,2,2-trifluoroethoxy]phenyl]-1,2,4-oxadiazol-3-yl]-3-methylphenyl]butanoic acid 856166-96-6P,  
 3-[4-[5-[3-Cyano-4-(2,2,2-trifluoroethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methylphenyl]butanoic acid 856167-09-4P 856167-14-1P  
 856167-19-6P, erythro-(±)-2,3-Dihydroxy-3-[4-[5-(3-cyano-4-isopropoxyphenyl)-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856167-21-0P, threo-(±)-2,3-Dihydroxy-3-[4-[5-(3-cyano-4-isopropoxyphenyl)-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856167-30-1P, 3-[4-[5-[3-Chloro-4-(isopropylthio)phenyl]-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of five-membered heterocycle-substituted benzenepropanoic and related acids as selective 51P1 (EDG1) receptor agonists)

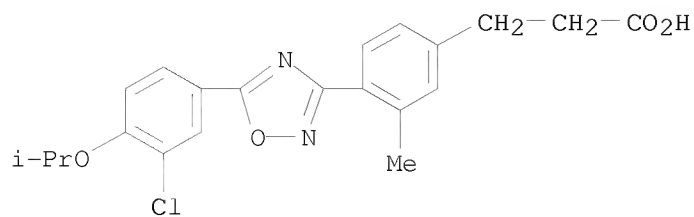
RN 856166-09-1 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-cyano-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



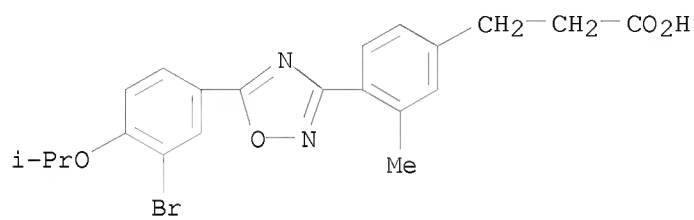
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CN Benzenepropanoic acid, 4-[5-[3-chloro-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



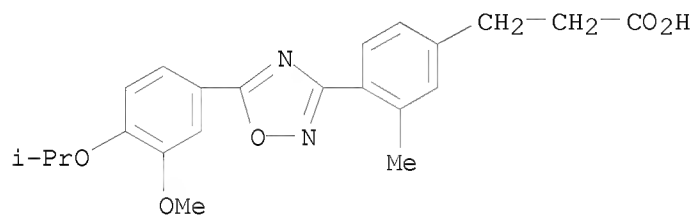
RN 856166-12-6 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-bromo-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



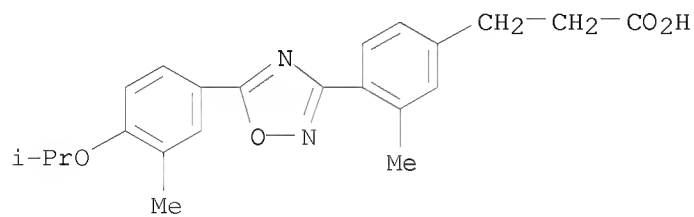
RN 856166-13-7 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-methoxy-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



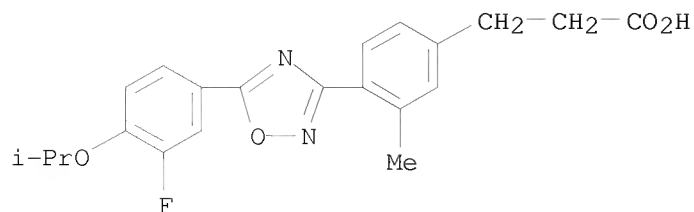
RN 856166-14-8 CAPLUS

CN Benzenepropanoic acid, 3-methyl-4-[5-[3-methyl-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)



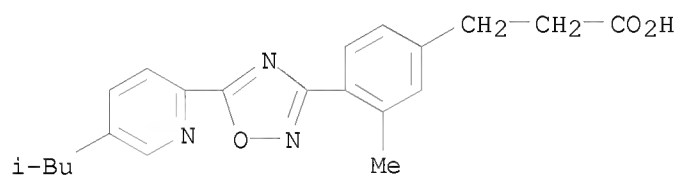
RN 856166-15-9 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-fluoro-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



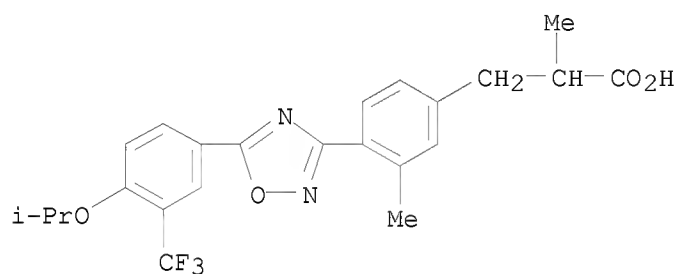
RN 856166-16-0 CAPLUS

CN Benzenepropanoic acid, 3-methyl-4-[5-[5-(2-methylpropyl)-2-pyridinyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)



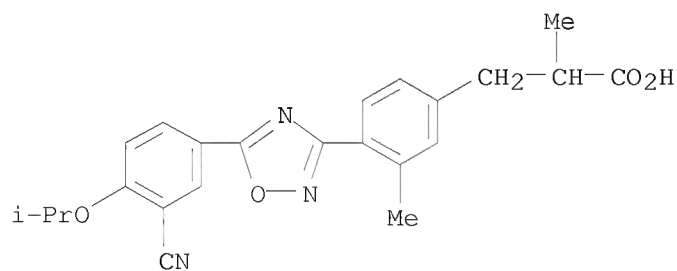
RN 856166-23-9 CAPLUS

CN Benzenepropanoic acid,  $\alpha$ ,3-dimethyl-4-[5-[4-(1-methylethoxy)-3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)



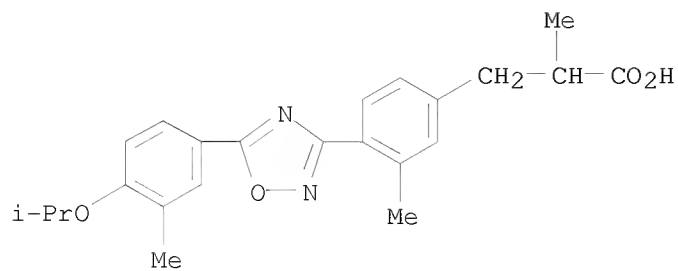
RN 856166-24-0 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-cyano-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]- $\alpha$ ,3-dimethyl- (CA INDEX NAME)

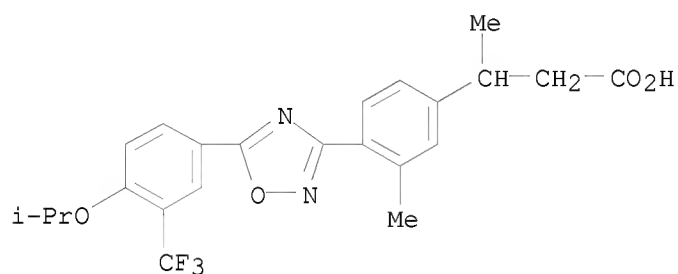


RN 856166-25-1 CAPLUS

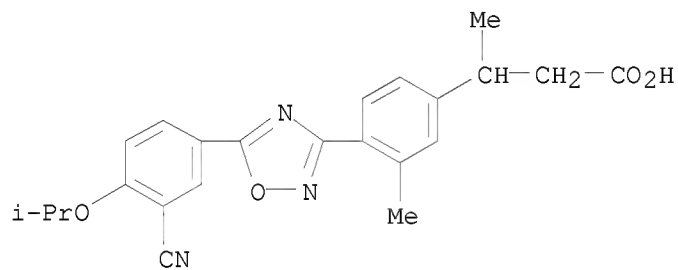
CN Benzenepropanoic acid,  $\alpha$ ,3-dimethyl-4-[5-[3-methyl-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)



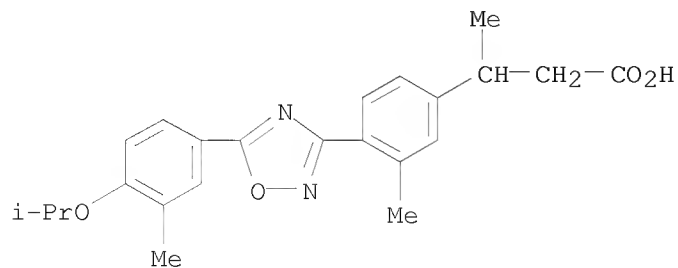
RN 856166-26-2 CAPLUS  
 CN Benzenepropanoic acid,  $\beta$ ,3-dimethyl-4-[5-[4-(1-methylethoxy)-3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)



RN 856166-27-3 CAPLUS  
 CN Benzenepropanoic acid, 4-[5-[3-cyano-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]- $\beta$ ,3-dimethyl- (CA INDEX NAME)

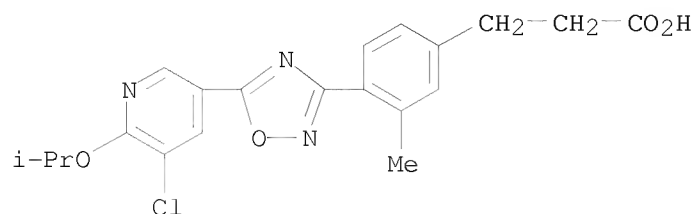


RN 856166-28-4 CAPLUS  
 CN Benzenepropanoic acid,  $\beta$ ,3-dimethyl-4-[5-[3-methyl-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)



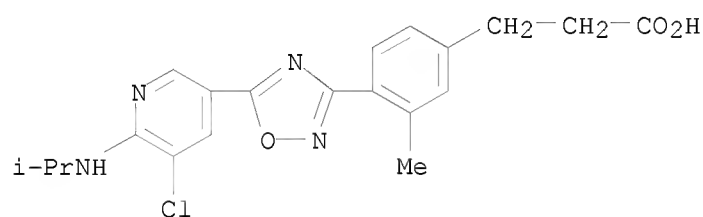
RN 856166-29-5 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-chloro-6-(1-methylethoxy)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



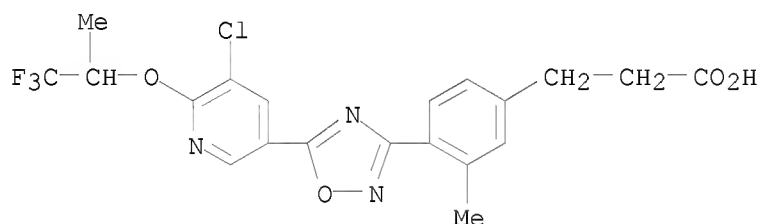
RN 856166-32-0 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-chloro-6-[(1-methylethyl)amino]-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



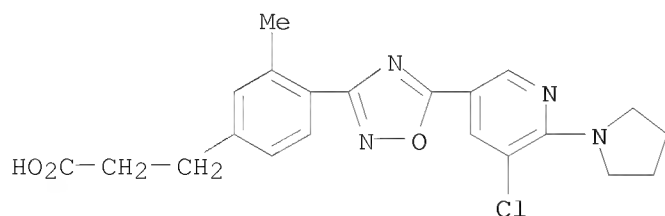
RN 856166-34-2 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-chloro-6-(2,2,2-trifluoro-1-methylethoxy)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



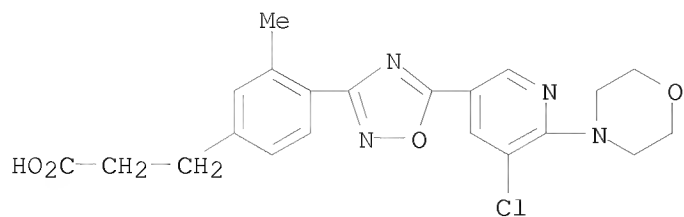
RN 856166-35-3 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-chloro-6-(1-pyrrolidinyl)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



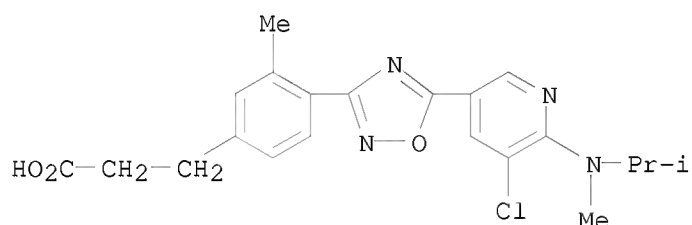
RN 856166-36-4 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-chloro-6-(4-morpholinyl)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



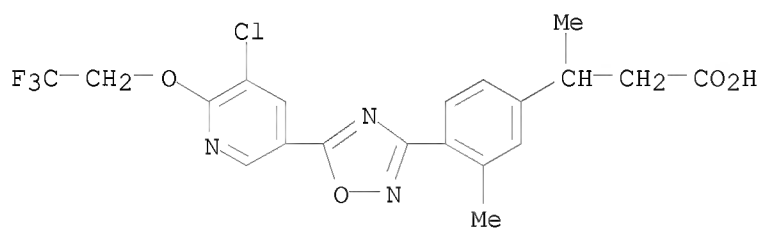
RN 856166-37-5 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-chloro-6-[methyl(1-methylethyl)amino]-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



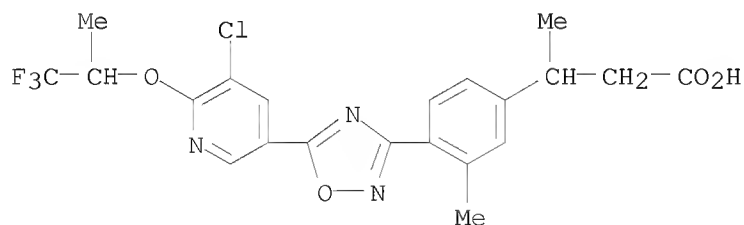
RN 856166-38-6 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-chloro-6-(2,2,2-trifluoroethoxy)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-β,3-dimethyl- (CA INDEX NAME)



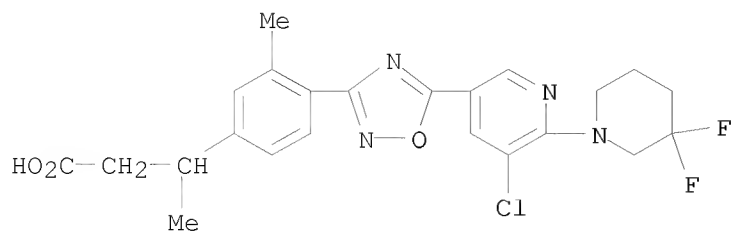
RN 856166-39-7 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-chloro-6-(2,2,2-trifluoro-1-methylethoxy)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-β,3-dimethyl- (CA INDEX NAME)



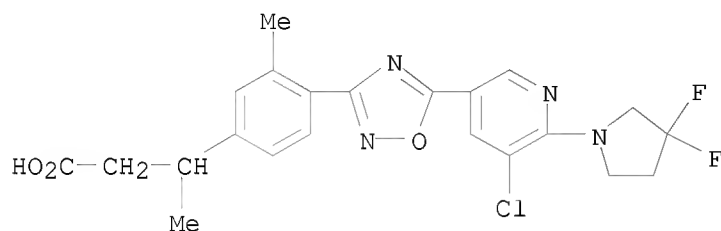
RN 856166-40-0 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-chloro-6-(3,3-difluoro-1-piperidinyl)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-β,3-dimethyl- (CA INDEX NAME)



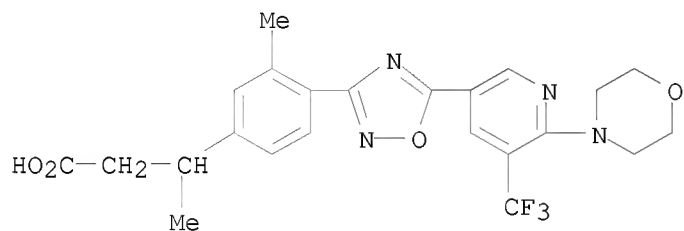
RN 856166-41-1 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-chloro-6-(3,3-difluoro-1-pyrrolidinyl)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-β,3-dimethyl- (CA INDEX NAME)



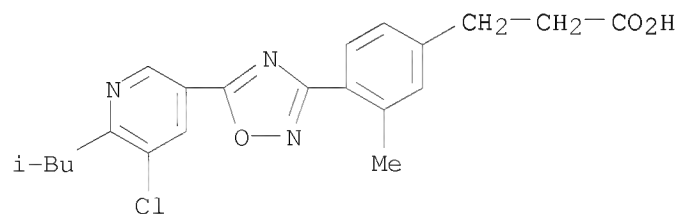
RN 856166-42-2 CAPLUS

CN Benzenepropanoic acid, β,3-dimethyl-4-[5-[6-(4-morpholinyl)-5-(trifluoromethyl)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)



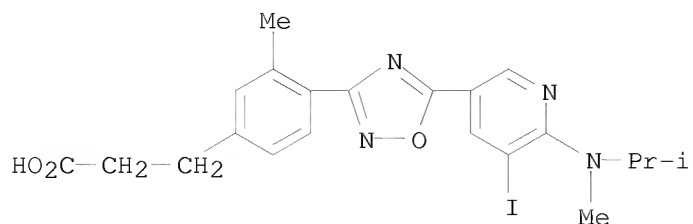
RN 856166-48-8 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-chloro-6-(2-methylpropyl)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



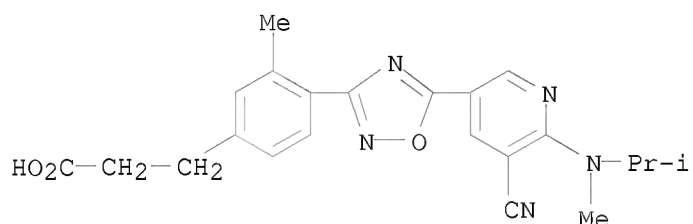
RN 856166-50-2 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-iodo-6-[methyl(1-methylethyl)amino]-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



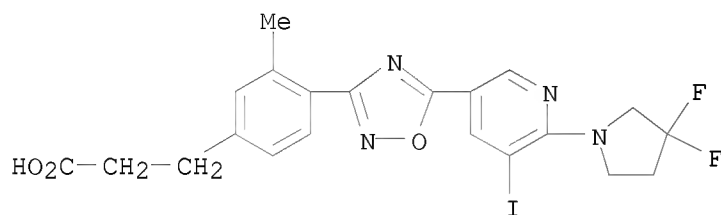
RN 856166-51-3 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-cyano-6-[methyl(1-methylethyl)amino]-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



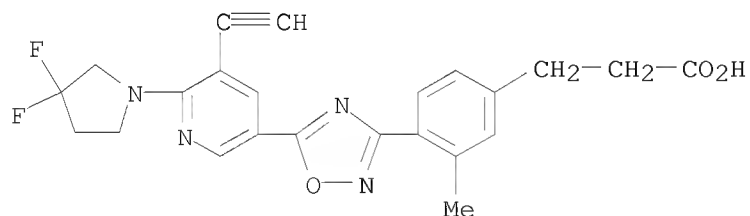
RN 856166-54-6 CAPLUS

CN Benzenepropanoic acid, 4-[5-[6-(3,3-difluoro-1-pyrrolidinyl)-5-iodo-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



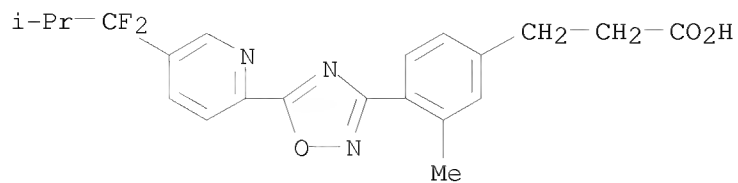
RN 856166-55-7 CAPLUS

CN Benzenepropanoic acid, 4-[5-[6-(3,3-difluoro-1-pyrrolidinyl)-5-ethynyl-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



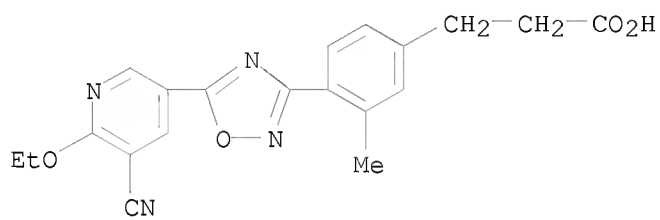
RN 856166-74-0 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-(1,1-difluoro-2-methylpropyl)-2-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



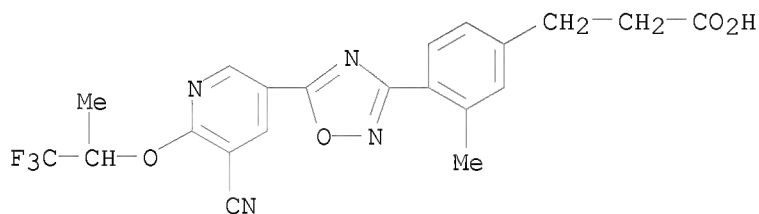
RN 856166-75-1 CAPLUS

CN Benzenepropanoic acid, 4-[5-(5-cyano-6-ethoxy-3-pyridinyl)-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



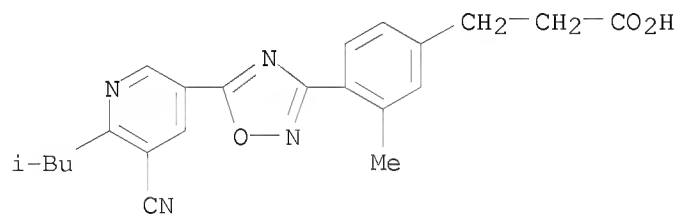
RN 856166-76-2 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-cyano-6-(2,2,2-trifluoro-1-methylethoxy)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



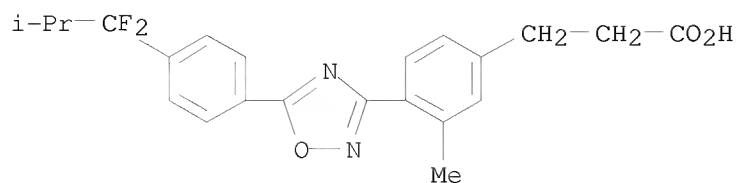
RN 856166-77-3 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-cyano-6-(2-methylpropyl)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



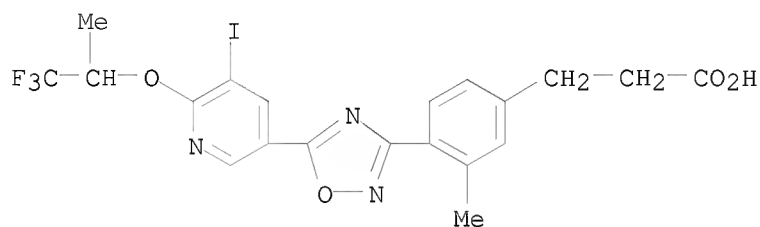
RN 856166-78-4 CAPLUS

CN Benzenepropanoic acid, 4-[5-[4-(1,1-difluoro-2-methylpropyl)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



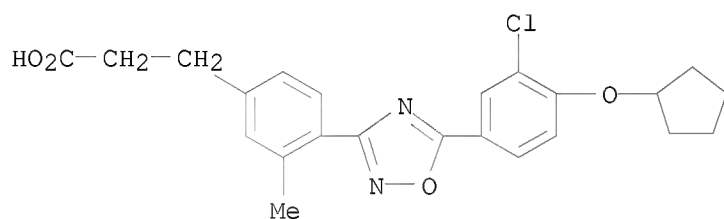
RN 856166-79-5 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-iodo-6-(2,2,2-trifluoro-1-methylethoxy)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



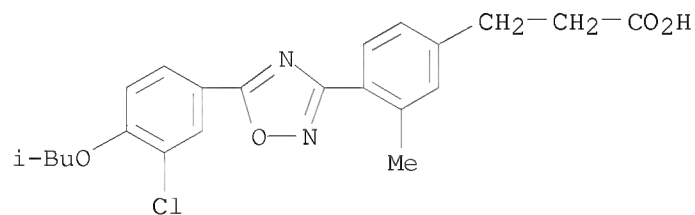
RN 856166-80-8 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-chloro-4-(cyclopentyloxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



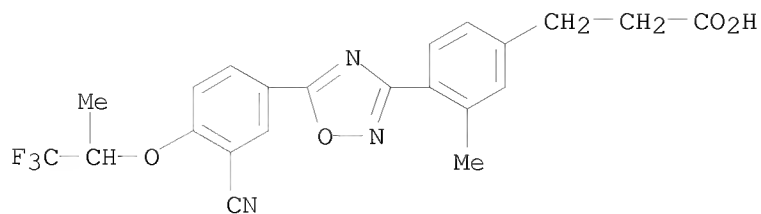
RN 856166-81-9 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-chloro-4-(2-methylpropoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

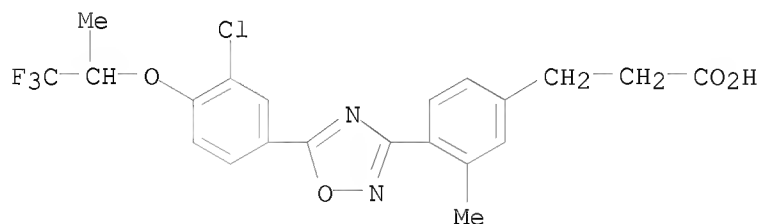


RN 856166-82-0 CAPLUS

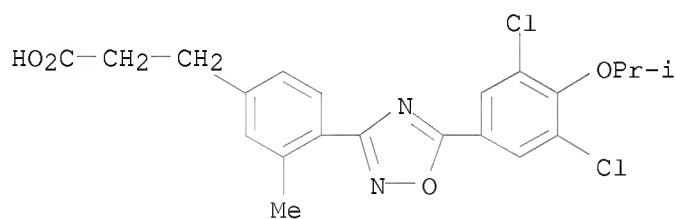
CN Benzenepropanoic acid, 4-[5-[3-cyano-4-(2,2,2-trifluoro-1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



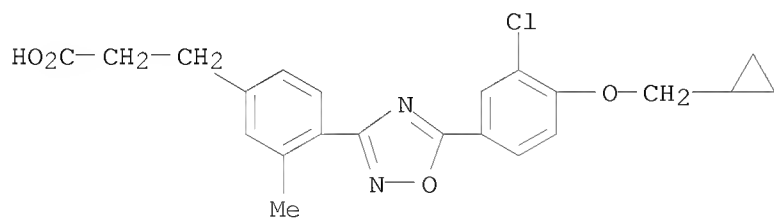
RN 856166-83-1 CAPLUS  
 CN Benzenepropanoic acid, 4-[5-[3-chloro-4-(2,2,2-trifluoro-1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



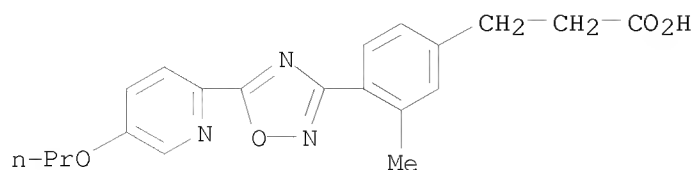
RN 856166-84-2 CAPLUS  
 CN Benzenepropanoic acid, 4-[5-[3,5-dichloro-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



RN 856166-85-3 CAPLUS  
 CN Benzenepropanoic acid, 4-[5-[3-chloro-4-(cyclopropylmethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

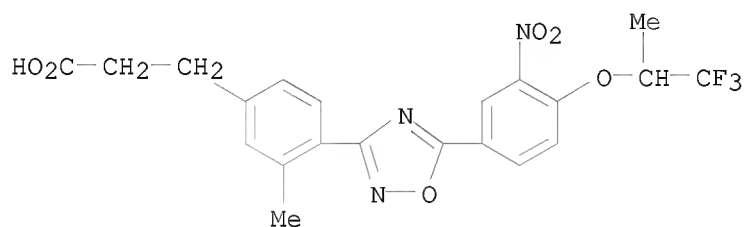


RN 856166-86-4 CAPLUS  
 CN Benzenepropanoic acid, 3-methyl-4-[5-(5-propoxy-2-pyridinyl)-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)



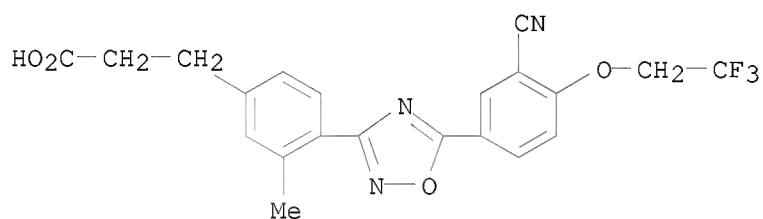
RN 856166-87-5 CAPLUS

CN Benzenepropanoic acid, 3-methyl-4-[5-[3-nitro-4-(2,2,2-trifluoro-1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)



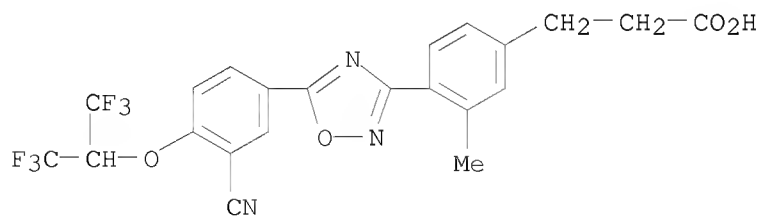
RN 856166-88-6 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-cyano-4-(2,2,2-trifluoroethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



RN 856166-89-7 CAPLUS

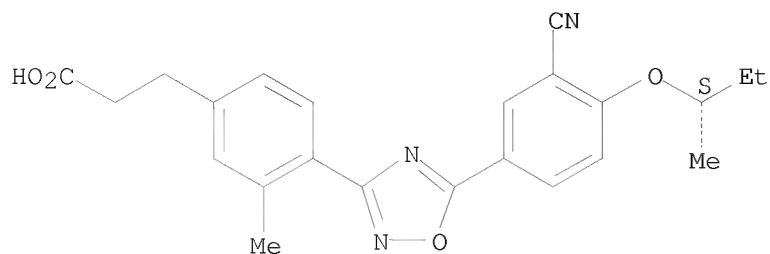
CN Benzenepropanoic acid, 4-[5-[3-cyano-4-[2,2,2-trifluoro-1-(trifluoromethyl)ethoxy]phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



RN 856166-90-0 CAPLUS

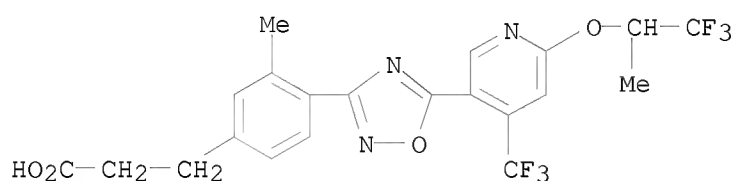
CN Benzenepropanoic acid, 4-[5-[3-cyano-4-[(1S)-1-methylpropoxy]phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

Absolute stereochemistry.



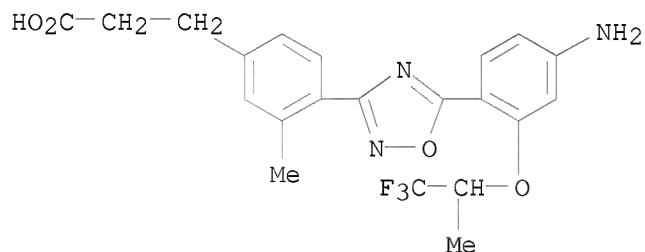
RN 856166-91-1 CAPLUS

CN Benzenepropanoic acid, 3-methyl-4-[5-[4-(trifluoromethyl)-6-(2,2,2-trifluoro-1-methylethoxy)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)



RN 856166-92-2 CAPLUS

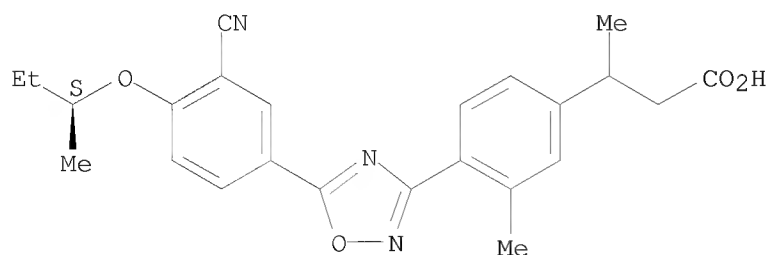
CN Benzenepropanoic acid, 4-[5-[4-amino-2-(2,2,2-trifluoro-1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



RN 856166-94-4 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-cyano-4-[(1S)-1-methylpropoxy]phenyl]-1,2,4-oxadiazol-3-yl]-β,3-dimethyl- (CA INDEX NAME)

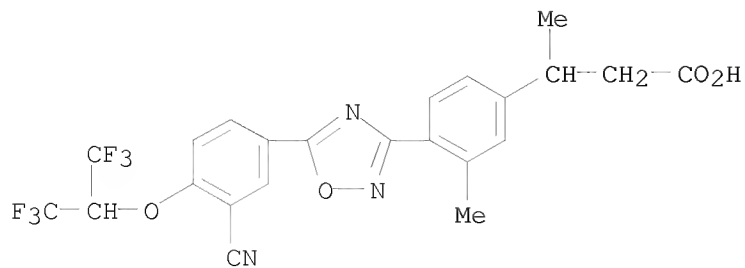
Absolute stereochemistry.



RN 856166-95-5 CAPLUS

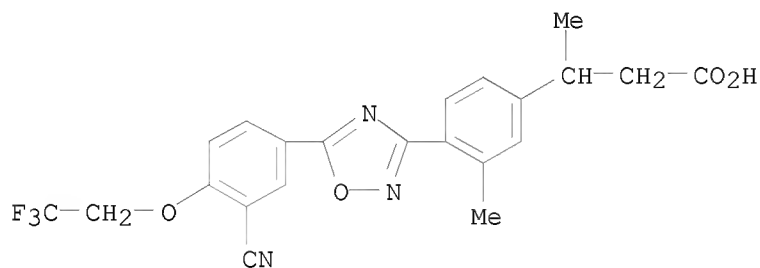
CN Benzenepropanoic acid, 4-[5-[3-cyano-4-[2,2,2-trifluoro-1-(trifluoromethyl)ethoxy]phenyl]-1,2,4-oxadiazol-3-yl]-β,3-dimethyl-

(CA INDEX NAME)



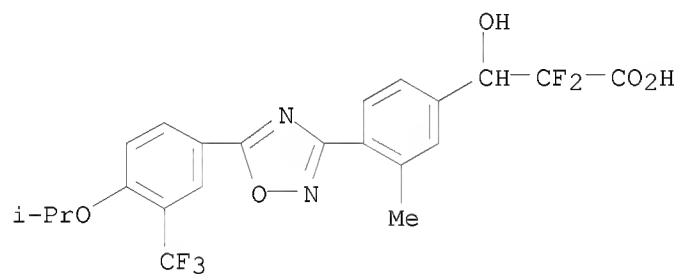
RN 856166-96-6 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-cyano-4-(2,2,2-trifluoroethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-β,3-dimethyl- (CA INDEX NAME)



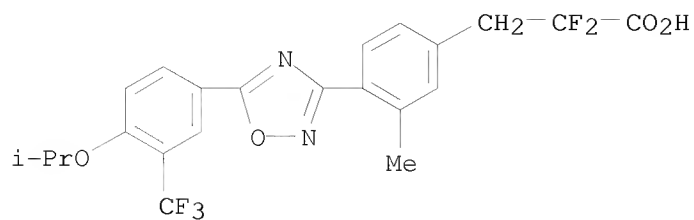
RN 856167-09-4 CAPLUS

CN Benzenepropanoic acid, α,α-difluoro-β-hydroxy-3-methyl-4-[5-[4-(1-methylethoxy)-3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)



RN 856167-14-1 CAPLUS

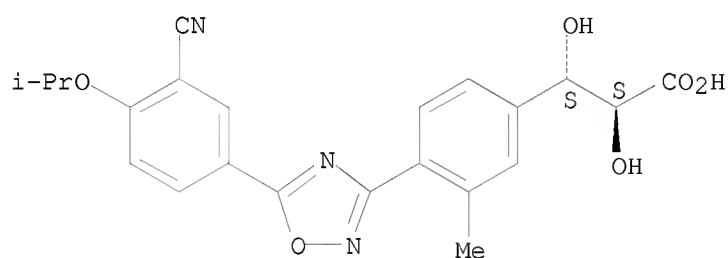
CN Benzenepropanoic acid, α,α-difluoro-3-methyl-4-[5-[4-(1-methylethoxy)-3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)



RN 856167-19-6 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-cyano-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]- $\alpha,\beta$ -dihydroxy-3-methyl-, ( $\alpha$ R, $\beta$ R)-rel- (CA INDEX NAME)

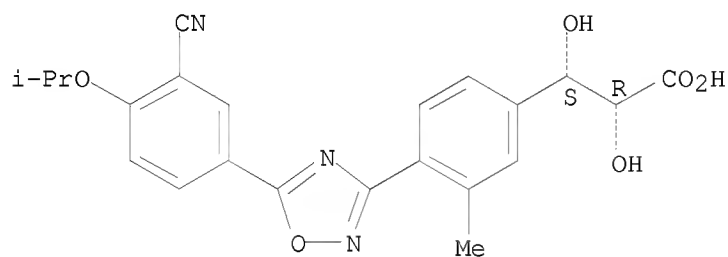
Relative stereochemistry.



RN 856167-21-0 CAPLUS

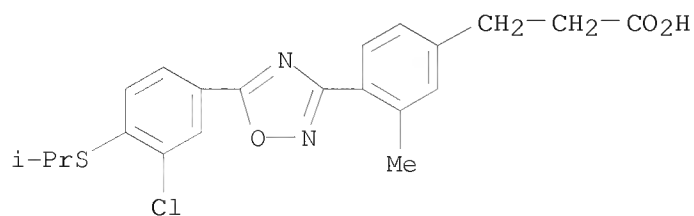
CN Benzenepropanoic acid, 4-[5-[3-cyano-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]- $\alpha,\beta$ -dihydroxy-3-methyl-, ( $\alpha$ R, $\beta$ S)-rel- (CA INDEX NAME)

Relative stereochemistry.



RN 856167-30-1 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-chloro-4-[(1-methylethyl)thio]phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



IT 856166-58-0P, 3-[4-[5-[6-(3,3-Difluoropyrrolidin-1-yl)-5-

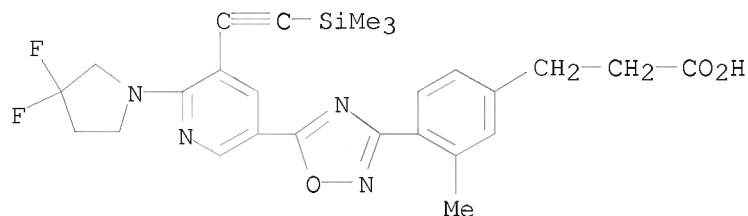
[(trimethylsilyl)ethynyl]pyridin-3-yl]-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of five-membered heterocycle-substituted benzenepropanoic and related acids as selective S1P1 (EDG1) receptor agonists)

RN 856166-58-0 CAPLUS

CN Benzenepropanoic acid, 4-[5-[6-(3,3-difluoro-1-pyrrolidinyl)-5-[2-(trimethylsilyl)ethynyl]-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

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404.10

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LOGINID:SSPTASXS1626

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FULL ESTIMATED COST

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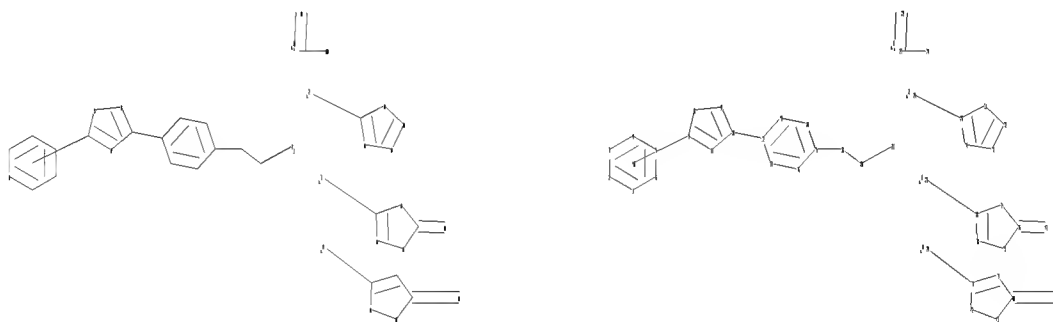
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predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

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Uploading C:\Program Files\STNEXP\Queries\123a.str



chain nodes :

21 22 23 24 25 27 29 43 44

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 26 28 30 31 32 33  
34 35 36 37 38 39 40 41 42

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ring/chain nodes :
18 20
chain bonds :
10-12 15-18 18-20 20-21 22-23 23-24 25-26 27-28 29-30 36-43 40-44
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-11 7-8 8-9 9-10 10-11 12-13 12-17 13-14
14-15 15-16 16-17 26-31 26-34 28-35 28-38 30-39 30-42 31-32 32-33 33-34
35-36 36-37 37-38 39-40 40-41 41-42
exact/norm bonds :
7-11 9-10 10-11 20-21 26-31 26-34 28-35 28-38 30-39 30-42 31-32 32-33
33-34 35-36 36-37 36-43 37-38 39-40 40-41 40-44 41-42
exact bonds :
7-8 8-9 10-12 15-18 18-20 25-26 27-28 29-30
normalized bonds :
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23-24
isolated ring systems :
containing 1 : 7 : 12 :

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G1:[*1],[*2],[*3],[*4]
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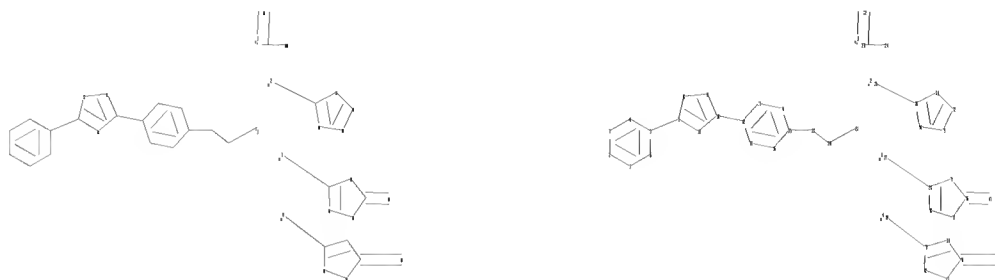
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21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:Atom 27:CLASS 28:Atom
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L8      STRUCTURE UPLOADED
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ring nodes :
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ring/chain nodes :
18 20
chain bonds :
5-7 10-12 15-18 18-20 20-21 22-23 23-24 25-26 27-28 29-30 36-43 40-44
ring bonds :
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35-36 36-37 37-38 39-40 40-41 41-42
exact/norm bonds :
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32-33 33-34 35-36 36-37 36-43 37-38 39-40 40-41 40-44 41-42
exact bonds :
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normalized bonds :
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23-24
isolated ring systems :
containing 1 : 7 : 12 :

```

```

G1:[*1],[*2],[*3],[*4]

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Match level :
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L9           STRUCTURE UPLOADED

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100.0% PROCESSED           12 ITERATIONS                   0 ANSWERS  
SEARCH TIME: 00.00.01

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100.0% PROCESSED           25 ITERATIONS                   5 ANSWERS  
SEARCH TIME: 00.00.01

L11           5 SEA SSS FUL L9

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